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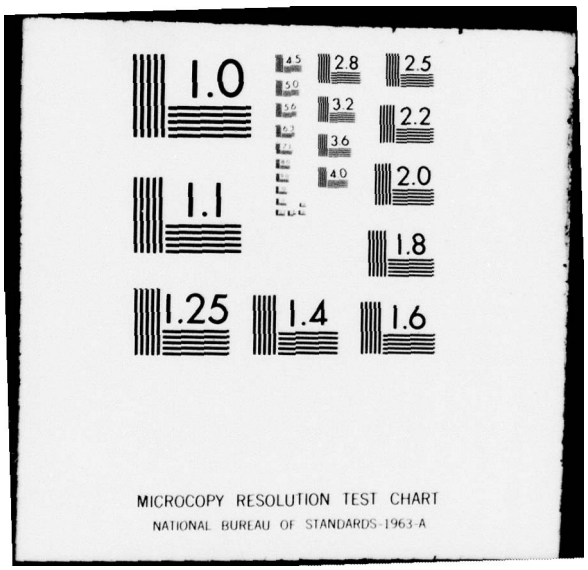
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6 CONFIDENCE LIMITS FOR THE OPTIMUM OF A SIMULATION RESPONSE FUNCTION

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by

10 Michael A. Crane and David W. Robinson

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1. INTRODUCTION AND SUMMARY

This paper deals with stochastic simulation in which the system being studied can be controlled to some extent by setting the value of an input parameter. The system response for a given input will vary from simulation run to simulation run due to uncontrolled and random factors; we thus consider the average or expected response. This is usually called the simulation response surface. Since our work here involves only a single variable the term response curve might be more appropriate.

The simulation "response" will generally be identified with some measure of system effectiveness and the analyst will want to maximize (or possibly minimize) the response by choosing the optimum value for the input parameter. More formally, if we denote the input parameter by λ and the expected response by $g(\lambda)$, we wish to solve the problem

$$\text{maximize} \quad g(\lambda) \quad . \tag{1}$$

The main difficulty in solving (1) is that $g(\lambda)$ can be evaluated only approximately due to the random factors in the simulation. If a simulation is carried out with the input parameter λ fixed at, say, a_1, the output from the run will be a confidence interval for which

$$\Pr\{A_1^1 \leq g(a_1) \leq A_1^2\} = 1 - \gamma_1 \quad , \tag{2}$$

where γ_1 is a user-specified value and $[A_1^1 , A_1^2]$ is the confidence interval. Such intervals depend on some assumed probability distribution (often normal) for the simulation outputs. We do not consider this underlying distribution more explicitly in this paper; the reader may refer to

[2] or [3] for some examples. We do require that intervals of the form (2) be found for each simulation run that is carried out.

The basic result of this paper requires as given a set of confidence intervals $\{A_i\}$ for the response surface values at fixed input parameter values $\{a_i\}$. (There are a variety of approaches for obtaining these confidence intervals, e.g. batch means, independent replications, autoregressive schemes, regenerative approach, etc.) These are used to obtain confidence intervals for the solution λ^* to (1), the optimum value $g(\lambda^*)$ and a joint confidence region for the point $(\lambda^*, g(\lambda^*))$, in the case where the response surface is quadratic, i.e.

$$g(\lambda) = z_1 + z_2\lambda + z_3\lambda^2 \quad . \tag{3}$$

The technique applied here is related to a confidence band methodology developed in a number of previous papers ([2] - [4]). The basic idea is to find the locus of the optima of all possible quadratic functions which pass simultaneously through each of the confidence intervals. The result (under some mild convexity assumptions) is a compact region whose x-axis dimensions give the required confidence interval for λ^*. The probability coverage of the final region is found by multiplying together the probabilities of the individual response surface confidence intervals.

The main drawback to our method is that the probability coverage of the confidence interval for the optimum may be quite low when many different parameter settings are used. By restricting ourselves to a quadratic response surface with a single input parameter, then, we may obtain results with but three or four observations while keeping the probability coverage

high. Moreover, the experience of workers in nonlinear programming and approximation theory indicates that a quadratic approximation is in many cases an entirely adequate representation for a smooth function over a restricted range. Thus, the assumed form (3) for $g(\lambda)$ is not necessarily restrictive.

The major strength of our technique is that it does not depend on the distribution of the simulation outputs in any way. In fact, probabilities are used only to find the probability of the final region by a simple multiplication. There is no need for regression, for equal variance assumptions or for distribution theory in analyzing simulation outputs.

Most other approaches to finding the optimum of a simulation response function involve carrying out a search over the parameter space; see [5] for a review and evaluation of work in this area. In our method no explicit attempt is made to determine the parameter setting for the next simulation run; rather, the emphasis is on using the information already obtained to determine where the optimum might be. The best use of the present work, then, would be to carry out an analysis of the final results of a simulation, perhaps using only the last 3-5 parameter settings.

The remainder of the paper is organized as follows: Section 2 presents the basic results and Section 3 consists of a numerical example. The final section reports on some straightforward extensions to the basic results and applies them to the numerical example.

2. BASIC RESULTS

Suppose that the response surface $g(\lambda)$ is as given by (3) and that simulation runs have been performed for the input parameter settings $\lambda = a_i$, $1 \le i \le n$, where $a_1 < \ldots < a_n$, $n \ge 3$. Suppose further that the simulation results are

$$\begin{aligned} A_1^1 \le g(a_1) \le A_1^2 \quad &\text{with probability} \quad 1 - \gamma_1 \ , \\ A_2^1 \le g(a_2) \le A_2^2 \quad &\text{with probability} \quad 1 - \gamma_2 \ , \\ &\ldots \\ A_n^1 \le g(a_n) \le A_n^2 \quad &\text{with probability} \quad 1 - \gamma_n \ . \end{aligned} \tag{4}$$

Assuming the simulation runs are independent, $g(\lambda)$ will satisfy all of the inequalities (4) with probability $(1 - \gamma_1)(1 - \gamma_2) \cdots (1 - \gamma_n) = 1 - \gamma$. (Alternatively, one might deal with simulations with dependent results as long as the probability $1 - \gamma$ may be found; this seems unlikely in practice, however, so we will not consider it further here.)

With probability $1 - \gamma$, then, $g(\lambda)$ must pass through the points (a_i , y_i) , $i = 1, \ldots n$, where $A_i^1 \le y_i \le A_i^2$. Consider the vector $y = (y_1, y_2, \ldots , y_n)$; if three of the components of y are fixed, the corresponding value of $z = (z_1, z_2, z_3)$ from (3) may be found and the remaining components of y evaluated. Assuming without loss of generality that the three fixed components are y_1, y_2, y_3 we have

$$z = \frac{(y_1 , y_2 , y_3)}{(a_3 - a_1)(a_2 - a_1)(a_3 - a_2)} \begin{bmatrix} (a_3 - a_2)a_2a_3 & a_2^2 - a_3^2 & a_3 - a_2 \\ (a_1 - a_3)a_1a_3 & a_3^2 - a_1^2 & a_1 - a_3 \\ (a_2 - a_1)a_1a_2 & a_1^2 - a_2^2 & a_2 - a_1 \end{bmatrix} \quad (5)$$

Thus (5) gives the coefficients of a quadratic function passing through the points (a_i, y_i) , $i = 1, 2, 3$. Note that the components of z in (5) are simple linear functions of the components of y . We may thus refer to "$z_1(y)$" , say, to indicate the result of (5) for a specific choice of the y vector.

When there are more than three simulation runs it is likely that not all possible choices for the components of y will be admissible since there may be no quadratic function passing through the specified points. We thus require that y be a member of the constraint set Y , where

$$Y = \{y \mid A_i^1 \leq y_i \leq A_i^2 \;\; ; \;\; i = 1, 2, 3 \; ; \quad A_i^1 \leq z_1(y) + z_2(y)a_i + z_3(y)a_i^2 \leq A_i^2 \;\; ; \; 3 < i \leq n\} . \quad (6)$$

Note that all of the constraints in Y are linear.

The optimum of the quadratic function (3) occurs at the parameter setting

$$\hat{\lambda} = - z_2/2z_3 \quad . \quad (7)$$

This will be a maximum as long as $z_3 < 0$, i.e. the response surface is strictly concave. We assume for the present that, in fact, $z_3 < 0$; dealing

with linear or convex response surfaces is discussed more fully in Section 4.3.

The $\hat{\lambda}$ value given by (7) may be viewed as a function of y just as z_2 and z_3 are. Substituting from (5) and simplifying yields

$$\hat{\lambda}(y) = \frac{(a_3^2 - a_2^2)y_1 - (a_3^2 - a_1^2)y_2 + (a_2^2 - a_1^2)y_3}{2(a_3 - a_2)y_1 - 2(a_3 - a_1)y_2 + 2(a_2 - a_1)y_3} \quad . \tag{8}$$

Thus (8) gives the optimum $\hat{\lambda}$ of a quadratic function passing through the points (a_i, y_i), $i = 1, 2, 3$. Since we have assumed $z_3 < 0$, $\hat{\lambda}(y)$ is a continuous bounded function over the closed compact set Y. Thus, as a function of $y \in Y$, $\hat{\lambda}(y)$ takes on a maximum $(\bar{\lambda})$ and a minimum $(\underline{\lambda})$ and all intervening values.

Now, given that $g(\lambda)$ is in fact quadratic and that it satisfies (4) (i.e., is contained by all of the simulation output confidence intervals) the optimum input parameter must lie in the closed interval $[\bar{\lambda}, \underline{\lambda}]$, where $\bar{\lambda} = \sup_{y \in Y} \hat{\lambda}(y)$ and $\underline{\lambda} = \inf_{y \in Y} \hat{\lambda}(y)$. Since the probability that (4) holds is just $1 - \gamma$, we have

$$\Pr\{\underline{\lambda} \leq \lambda^* \leq \bar{\lambda}\} \leq 1 - \gamma \quad . \tag{9}$$

This is the desired confidence interval for λ^*. (The inequality results from the observation that the optimal parameter may lie in the given interval even in cases where the quadratic does not lie within the simulation output confidence interval.)

Finding $\underline{\lambda}$ and $\bar{\lambda}$ is quite straightforward. Examining the gradient vector found by differentiating (8):

$$\nabla_y \hat{\lambda}(y) = \frac{(a_2 - a_1)(a_3 - a_2)(a_3 - a_1)}{2[(a_3 - a_2)y_1 - (a_3 - a_1)y_2 + (a_2 - a_1)y_3]^2} \begin{bmatrix} y_3 - y_2 \\ y_1 - y_3 \\ y_2 - y_1 \end{bmatrix}$$

shows that the fraction will always be positive, since the denominator is proportional to z_3^2 . Thus, when two of the first three components of y are fixed the direction of change of $\hat{\lambda}(y)$ is constant. (The rate of change varies but not the direction.) $\hat{\lambda}(y)$ may thus be increased, say, by changing the unfixed y component until one of the constraints in (6) becomes binding; this shows that both $\underline{\lambda}$ and $\bar{\lambda}$ occur at extreme points of the set Y , i.e. three of the simulation output confidence interval inequalities (4) will be binding.

Now suppose that λ is fixed at some point $[\underline{\lambda}, \bar{\lambda}]$. We know that there is at least one y vector such that $\hat{\lambda}(y) = \lambda$, i.e. the quadratic function passing through (a_i , y_i) , $1 \leq i \leq n$, has its optimum at λ . In general there will be a set of such vectors and the maximum response value $g(\lambda)$ will vary as different y values are selected. Denote by $\hat{g}(\lambda ; y)$ this maximum and define the functions

$$\underline{g}(\lambda) = \inf_{\substack{\hat{\lambda}(y) = \lambda \\ y \in Y}} \hat{g}(\lambda ; y) \qquad (10)$$

$$\overline{g}(\lambda) = \sup_{\substack{\hat{\lambda}(y) = \lambda \\ y \in Y}} \hat{g}(\lambda ; y) \tag{11}$$

These functions then depict a joint confidence region for the point $(\lambda^*, g(\lambda^*))$, i.e.

$$\Pr\{(\lambda^*, g(\lambda^*)) \in G\} \geq 1 - \gamma \tag{12}$$

where

$$G = \{(\lambda, g) \mid \underline{\lambda} \leq \lambda \leq \overline{\lambda} \; ; \; \underline{g}(\lambda) \leq g \leq \overline{g}(\lambda)\} \; .$$

This follows just as for (9).

Now (10) and (11) are linear programs for fixed λ . We show this as follows: the first constraint $(\hat{\lambda}(y) = \lambda)$ may be rewritten as $-z_2(y) = 2\lambda z_3(y)$ according to (7); simplifying using (5) yields

$$y_2 = \frac{(a_3 - a_2)(a_3 + a_2 - 2\lambda)}{(a_3 - a_1)(a_3 + a_1 - 2\lambda)} y_1 + \frac{(a_2 - a_1)(a_2 + a_1 - 2\lambda)}{(a_3 - a_1)(a_3 + a_1 - 2\lambda)} y_3 \; . \tag{13}$$

(13) shows that as y_1 and y_3 change, y_2 shifts so as to keep the optimum fixed at λ . The value of $\hat{g}(\lambda ; y)$ is given by $z_1(y) - z_3(y)\lambda^2$; substituting from (5) and (13) gives

$$\hat{g}(\lambda\,;\,y) \;=\; \frac{(a_3-\lambda)^2}{(a_3-a_1)(a_3+a_1-2\lambda)}\,y_1 \;-\; \frac{(\lambda-a_1)^2}{(a_3-a_1)(a_3+a_1-2\lambda)}\,y_3 \qquad (14)$$

The solution to (10) and (11) will then have two components of y (say, y_1 and y_3) at their bounds, with the third component y_2 determined by the optimality constant $\hat{\lambda}(y) = \lambda$, or (13).

This analysis must be repeated when $a_3 + a_2 - 2\lambda = 0$, i.e. λ is at the midpoint of $[a_1, a_3]$. (Note that this point may not be in $[\underline{\lambda}, \bar{\lambda}]$.) In this case, we obtain

$$y_1 \;=\; y_3 \qquad (15)$$

$$\hat{g}\left(\frac{a_3+a_1}{2}\,;\,y\right) \;=\; y_1 + \frac{(a_3-a_1)^2}{4(a_3-a_2)(a_2-a_1)}\,(y_2-y_1)\;. \qquad (16)$$

There are two alternatives for computing the bound functions. If this is to be done by "brute force" (either manually or with a computer) it is suggested that the analyst select each possible set of two extreme points in y and investigate the behavior of $\hat{g}(\lambda\,;\,y)$ as a third component of y is varied and λ is adjusted to maintain optimality; this approach is feasible for perhaps three or four observations. For more observations, it is suggested that the simple linear programs (10) and (11) be solved directly for different values of λ.

Unfortunately, it is also tedious to obtain a confidence region for $g(\lambda^*)$ alone. The values

$$\underline{g} = \inf_{\lambda \in [\underline{\lambda}, \overline{\lambda}]} g(\lambda) \tag{17}$$

$$\overline{g} = \sup_{\lambda \in [\underline{\lambda}, \overline{\lambda}]} \overline{g}(\lambda) \tag{18}$$

will satisfy

$$\Pr\{\underline{g} \leq g(\lambda^*) \leq \overline{g}\} \geq 1 - \gamma \tag{19}$$

just as for (9) and (12). The simplest way to solve (17) and (18) is by inspection from the $\underline{g}(\lambda)$, $\overline{g}(\lambda)$ plots.

The values of $\underline{g}$ and $\overline{g}$ do not in general occur at an extreme point of y although they often seem to. It is suggested, therefore, that the $(\hat{\lambda}(y), \hat{g}(\hat{\lambda}(y); y))$ values be plotted for each feasible y vector with three or more of its components fixed at their upper or lower bounds. This will always yield the values for $\underline{\lambda}$ and $\overline{\lambda}$ and will often yield the values for $\underline{g}$ and $\overline{g}$.

3. NUMERICAL EXAMPLE

In this section we present a worked-out example as an aid to understanding the analysis of the preceding section. The following data are given:

i	a_i	A_i^1	A_i^2	γ_i
1	-1	1	2	.02
2	0	4	5	.02
3	1	1	4	.01

Thus, for example, $[1, 2]$ is a 98% confidence interval for $g(\lambda)$ at $\lambda = -1$. The probability content of the final region is $(.98)(.98)(.99) = .95$ approximately. The coefficients z_i are given by

$$\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & -1 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} y_2 \\ \frac{1}{2}(y_3 - y_1) \\ \frac{1}{2}(y_1 - 2y_2 + y_3) \end{bmatrix} ,$$

while the function $\hat{\lambda}(y)$ is

$$\hat{\lambda}(y) = \frac{y_1 - y_3}{2y_1 - 4y_2 + 2y_3}$$

The set Y is given by $y = \{y \mid 1 \le y_1 \le 2 , 4 \le y_2 \le 5 , 1 \le y_3 \le 4\}$. The bounds on λ^* are then readily found by observing the extreme points of the set y :

$$\underline{\lambda} = -\frac{1}{10} \quad , \qquad \text{for} \qquad y = \begin{bmatrix} 2 \\ 4 \\ 1 \end{bmatrix}$$

$$\overline{\lambda} = \frac{1}{2} \quad , \qquad \text{for} \qquad y = \begin{bmatrix} \text{any} \\ 4 \\ 4 \end{bmatrix}$$

For any $\lambda \in \left[-\frac{1}{10} , \frac{1}{2}\right]$ and $y \in Y$, we have, for optimality,

$$y_2 = \frac{2\lambda - 1}{4\lambda} y_1 + \frac{2\lambda - 1}{4\lambda} y_3 \ ,$$

$$\hat{g}(\lambda ; y) = \frac{(1+\lambda)^2}{4\lambda} y_3 - \frac{(1-\lambda)^2}{4\lambda} y_1 \quad (\lambda \neq 0) \ ,$$

$$\hat{g}(0 ; y) = y_2 \ .$$

The resulting $\underline{g}(\lambda)$, $\overline{g}(\lambda)$ functions are obtained, in this case, by examining the values of $\hat{g}(\lambda ; y)$ when two components of y are set at the various extreme points and the third component is allowed to vary. Taking the minimum and maximum values for each λ yields:

$$g(\lambda) = \frac{2\lambda^2 + 8\lambda + 4}{2\lambda + 1} \quad -\frac{1}{10} \leq \lambda \leq \frac{1}{2} \quad (y_1 = 2 \ , \ y_2 = 4) \qquad (20)$$

$$\bar{g}(\lambda) = \begin{cases} \dfrac{\lambda^2 - 6\lambda + 1}{-4\lambda} & -\frac{1}{10} \le \lambda \le \frac{1}{14} \quad (y_1 = 2,\ y_3 = 1) \\ \dfrac{4\lambda^2 - 10\lambda + 5}{1 - 2\lambda} & -\frac{1}{14} \le \lambda \le 0 \quad (y_2 = 5,\ y_3 = 1) \\ \dfrac{4\lambda^2 + 10\lambda + 5}{1 + 2\lambda} & 0 \le \lambda \le \frac{3}{10} \quad (y_1 = 1,\ y_2 = 5) \\ \dfrac{3\lambda^2 + 10\lambda + 3}{4\lambda} & \frac{3}{10} \le \lambda \le \frac{1}{2} \quad (y_1 = 1,\ y_3 = 4) \end{cases} \tag{21}$$

The segments of each function are annotated with the values of the y vector components which remain fixed. The functions are plotted in Figure 1. Note the characteristic (and unusual) shape of the joint confidence region for $(\lambda^*, g(\lambda^*))$. Figure 1 shows the upper and lower confidence bands for the response $g(\lambda)$; see [3] for details.

By inspection we find that

$$\underline{g} = 4 \quad \text{for} \quad \lambda = 0$$

$$\bar{g} = 5.225 \quad \text{for} \quad \lambda = 3/10$$

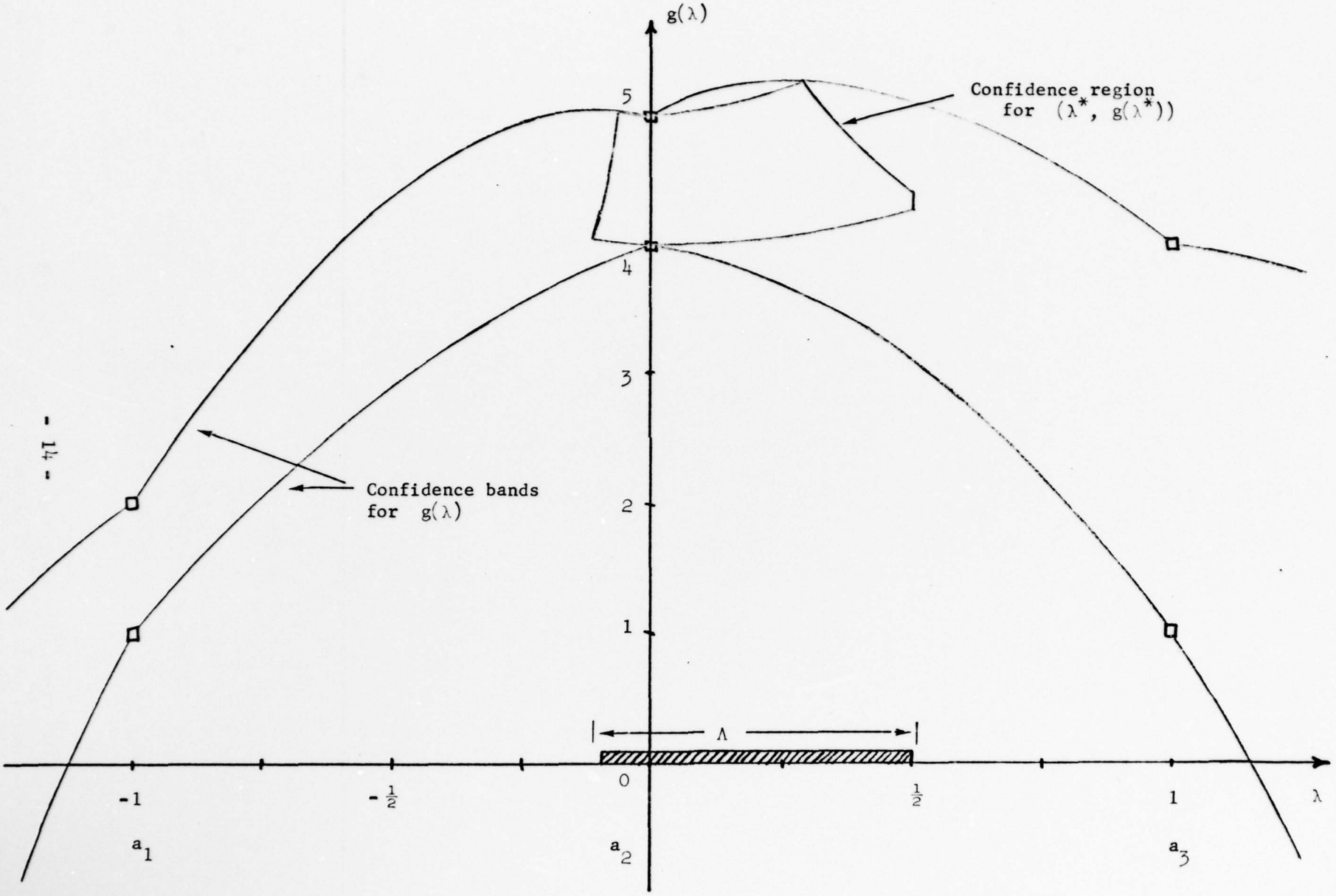

Figure 1. Confidence bands for $g(\lambda)$ and confidence region for $(\lambda^*, g(\lambda^*))$ for numerical example.

4. SOME EXTENSIONS

In this Section we take up a few obvious extensions to the work of Section 2. These are: dealing with a quadratic function with more than three simulation outputs, handling non-concavity and selection of good confidence interval widths at each base point. Extensions to the numerical example of Section 3 are also presented.

4.1 Additional Observations

Suppose that a fourth parameter setting $a_4 = 1/2$ is chosen for our numerical example and that, with probability .98, $4 \leq g(1/2) \leq 5$. Including this additional observation decreases the probability of our final results to about .93; this points up the major disadvantage of adding new observations to an existing solution.

The various optimization problems solved in Section 3 must be augmented by adding the constraints

$$4 \leq -\frac{1}{8} y_1 + \frac{3}{4} y_2 + \frac{3}{8} y_3 \leq 5 \quad .$$

When this is done, we obtain

$$\underline{\lambda} = -1/20 \quad \text{for} \quad y = \begin{bmatrix} 2 \\ 5 \\ 4/3 \\ 4 \end{bmatrix}$$

$$\overline{\lambda} = 1/2 \quad \text{for} \quad y = \begin{bmatrix} 2 \\ 4 \\ 4 \\ 4\ 1/4 \end{bmatrix}$$

The functions $\underline{g}(\lambda)$ and $\bar{g}(\lambda)$ can also be found; their form is similar to (20) and (21) and they are plotted in Figure 2. The results for the optimum value bounds are

$$\underline{g} = 4\ 1/2 \quad \text{for} \quad \lambda = 1/4 \ ,$$

$$\bar{g} = 5\ 1/6 \quad \text{for} \quad \lambda = 1/4 \ .$$

It is instructive to consider the reduction in size of the various confidence regions when the fourth observation is added. The intervals for λ^* and $g(\lambda^*)$ are reduced in length by 8.3% and 8.2%, respectively. By performing a somewhat tedious integration, one may find that the joint confidence region on $(\lambda^*, g(\lambda^*))$ is reduced in area by 24%.

4.2 Interval Width Selection

Instead of performing a simulation with an entirely new parameter setting as in the previous subsection, one may choose to perform more replications at one of the existing settings in order to narrow the confidence interval $[A_i^1, A_i^2]$ at that point. Note that this procedure leaves the probability content of the resulting confidence regions unchanged. Alternatively, it is usually possible to narrow any of the original confidence intervals if one is willing to accept the resulting decrease in the probability content of the final results. We thus consider the selection of a set of good widths for the $[A_i^1, A_i^2]$ intervals.

Because of the complex expressions that arise if one allows too much generality, it is difficult to give robust rules for choosing the interval

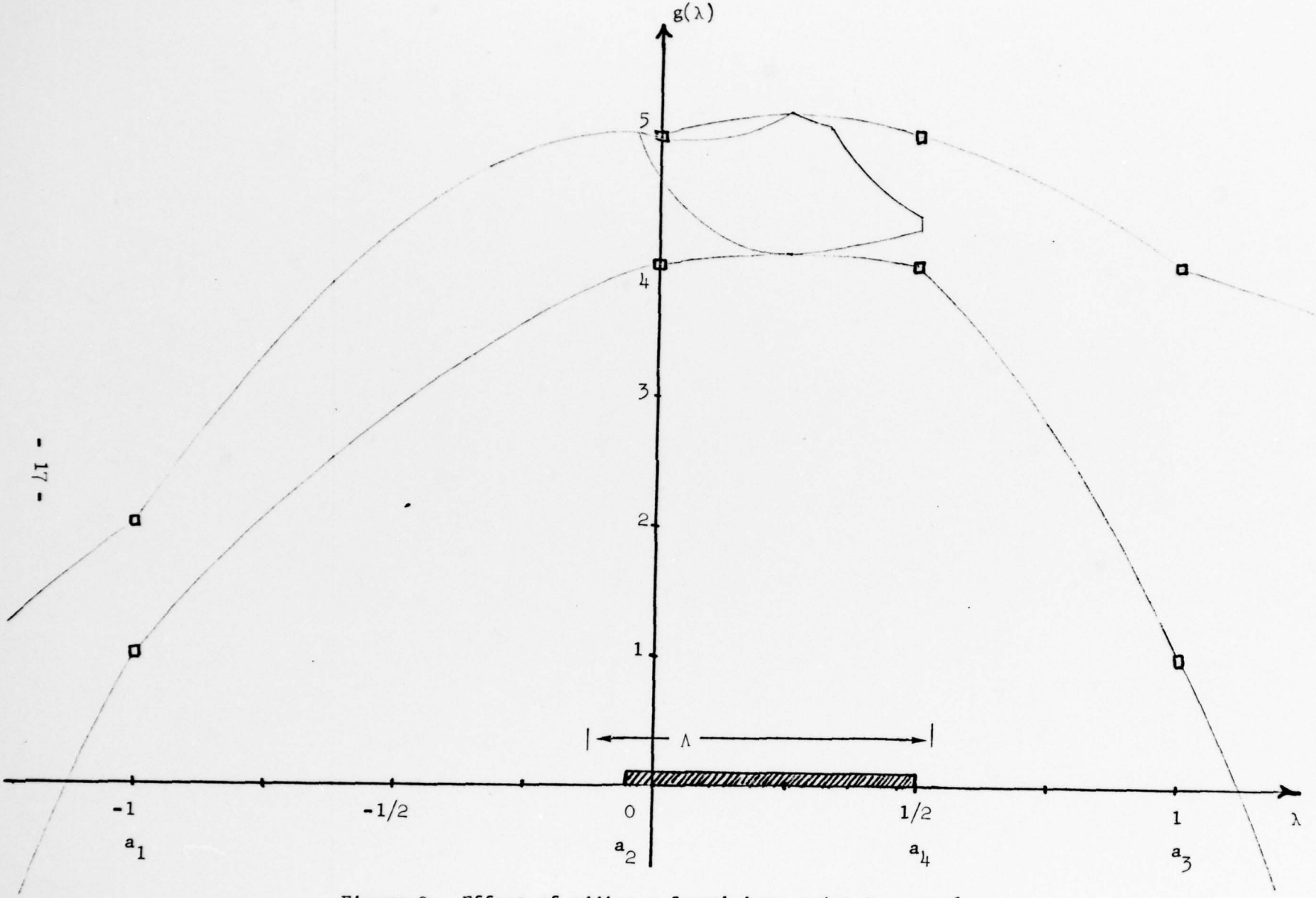

Figure 2. Effect of adding a fourth base point to example.

widths. Intuitively, it seems best to select all with about the same width, or else with about the same probability coverage. In order to consider this matter more concretely, we shall look more closely at the example of Section 3.

If the additional simulation replications carried out at $\lambda = a_4$ in Section 4.1 had been run instead for $\lambda = a_3$, the confidence interval $[A_3^1, A_3^2]$ would be based on twice as many observations and would thus be about 70.7% as wide as the original interval with the same probability coverage. The calculations of Section 3 were repeated, therefore, with $A_3^1 = 1.5$ and $A_3^2 = 3.5$; the results are plotted in Figure 3 and are summarized below:

$$\underline{\lambda} = \frac{1}{18} \qquad \text{for} \qquad y = \begin{bmatrix} 2 \\ 4 \\ 1\frac{1}{2} \end{bmatrix}$$

$$\overline{\lambda} = \frac{5}{14} \qquad \text{for} \qquad y = \begin{bmatrix} 1 \\ 4 \\ 3\frac{1}{2} \end{bmatrix}$$

$$\underline{g} = 4 \qquad \text{for} \qquad \lambda = 0$$

$$\overline{g} = 5\,{}^{25}/_{176} \qquad \text{for} \qquad \lambda = {}^{5}/_{22} \quad .$$

The size of $[\underline{\lambda}, \overline{\lambda}]$ thus decreases by 31% and of $[\underline{g}, \overline{g}]$ by 6.8%; the area of the $(\lambda^*, g(\lambda^*))$ region decreases by 41%. It may thus be concluded that in this instance it is preferable to narrow the third confidence interval than to take additional observations at some other point.

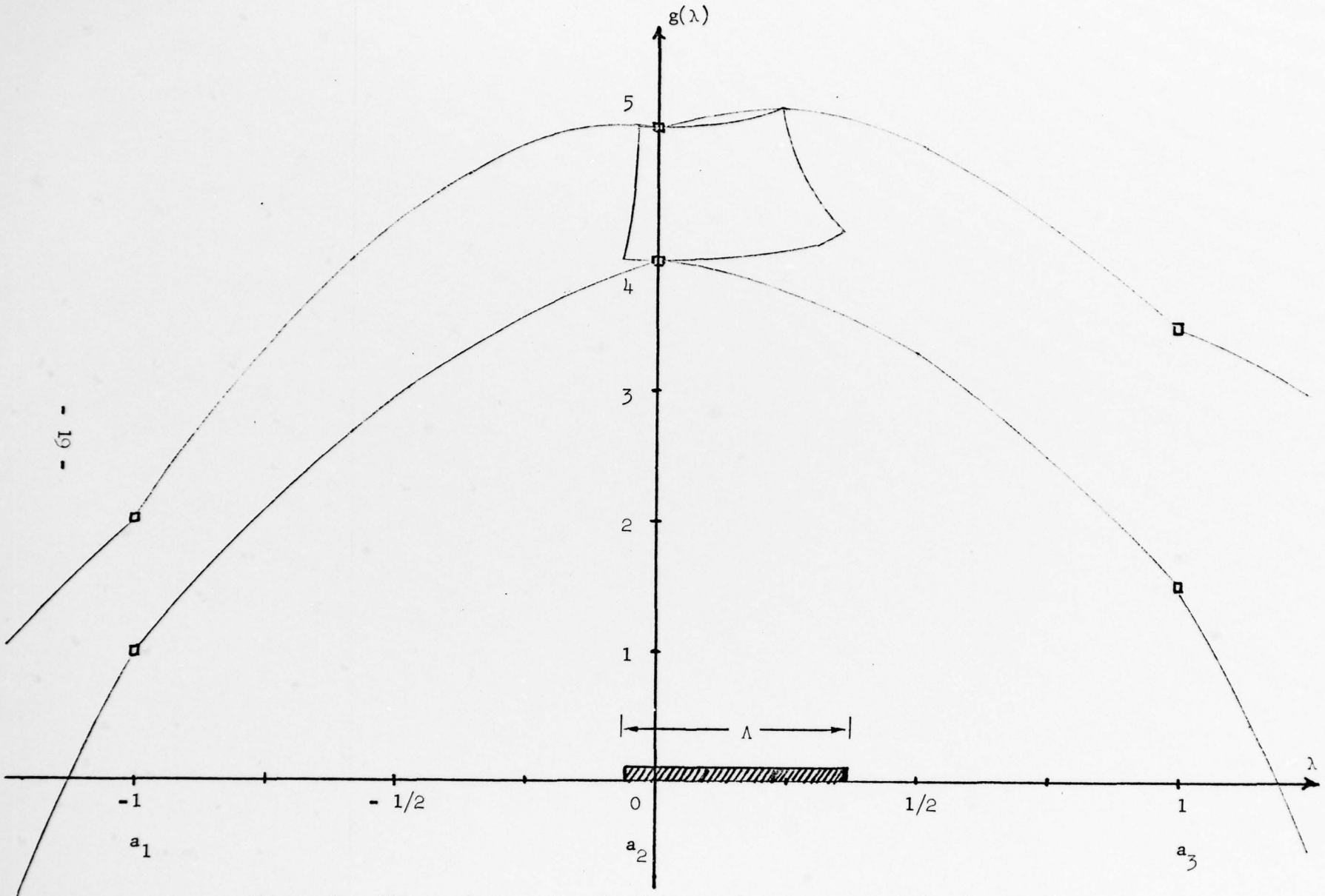

Figure 3. Effect of narrowing the third confidence interval in the example.

To pursue the matter further, we investigate how the widths of the $[\underline{\lambda}, \overline{\lambda}]$ and $[\underline{g}, \overline{g}]$ confidence intervals change as the $[A_3^1, A_3^2]$ interval changes. We assume that

$$A_3^1 = 2^{1/2} - \delta \quad , \qquad A_3^2 = 2^{1/2} + \delta \quad .$$

The resulting widths are plotted in Figure 4. Note that when $\delta = 3^{1/2}$ in this case, the vector $y = \begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix}$ yields a linear function; the upper bound $\overline{\lambda}$ thus approaches $+\infty$ as δ increases.

If we further assume that the simulation response at $\lambda = a_3$ has a normal distribution (on an approximately normal distribution) we can plot the sizes of the two confidence intervals against their probability coverage; note that since the a_1 and a_2 intervals do not change in this case, the maximum probability is $(.98)^2 = .9604$. The result is shown in Figure 5. Note the sharp upward turn at a point corresponding to $1 - \gamma = .94$, i.e. $\gamma_3 \approx .02$.

Both Figures 4 and 5 lend some wieght to our previous observation that the "best" confidence regions for λ^* and $g(\lambda^*)$ result when the absolute widths of the simulation output confidence intervals are about the same. We must qualify this statement somewhat when the parameter settings are not evenly spaced, since a greater width is acceptable for parameter settings which are relatively distant from the optimum.

4.3 Non-Concave Functions

When the value of $z_3(y)$ found from (5) is not negative, the resulting $g(\lambda)$ function becomes unbounded as $\lambda \to \pm \infty$. As we saw in Section 4.2, this will cause either $\underline{\lambda}$ or $\overline{\lambda}$ or both to become unbounded as well.

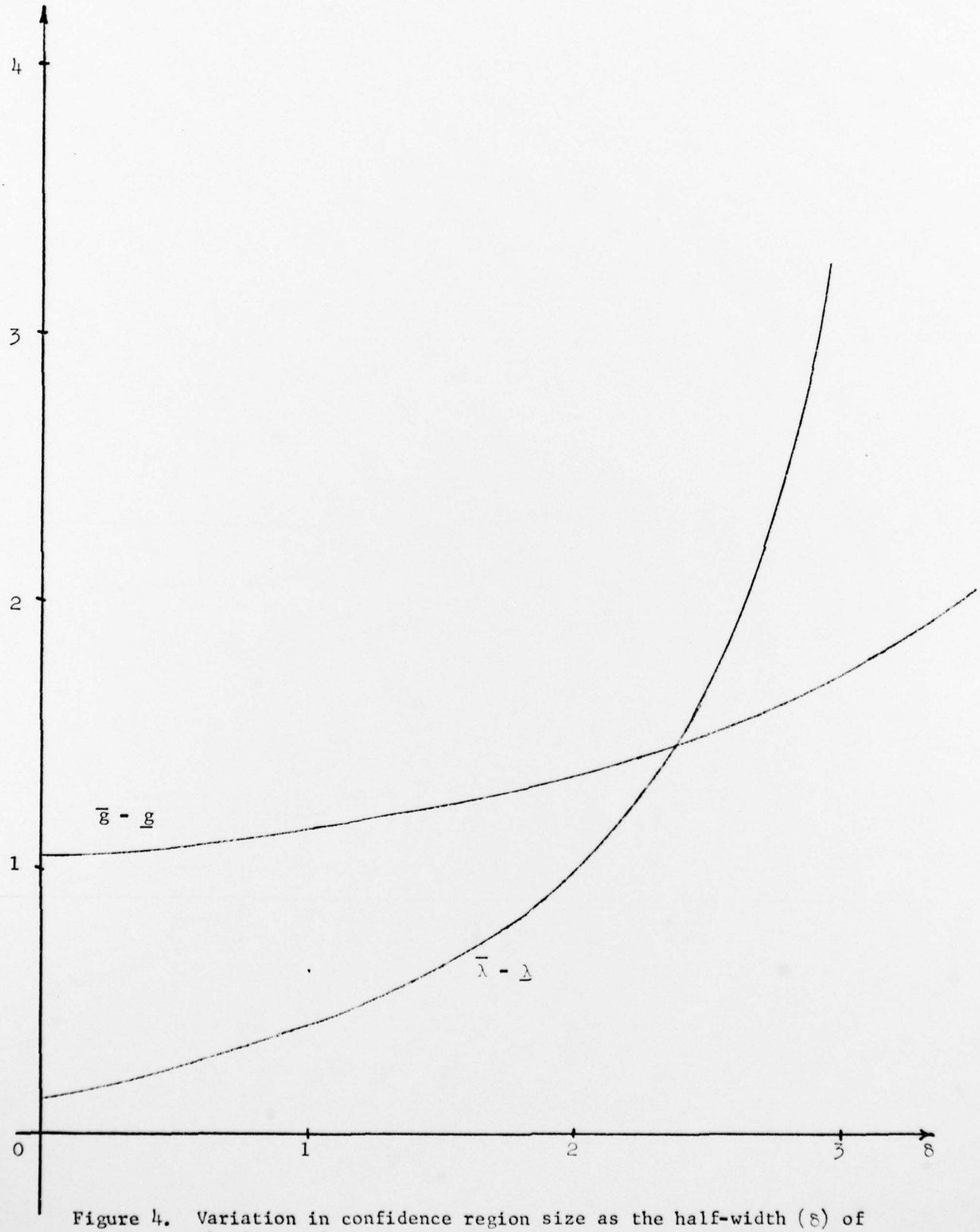

Figure 4. Variation in confidence region size as the half-width (δ) of the interval at $\lambda = a_3$ changes.

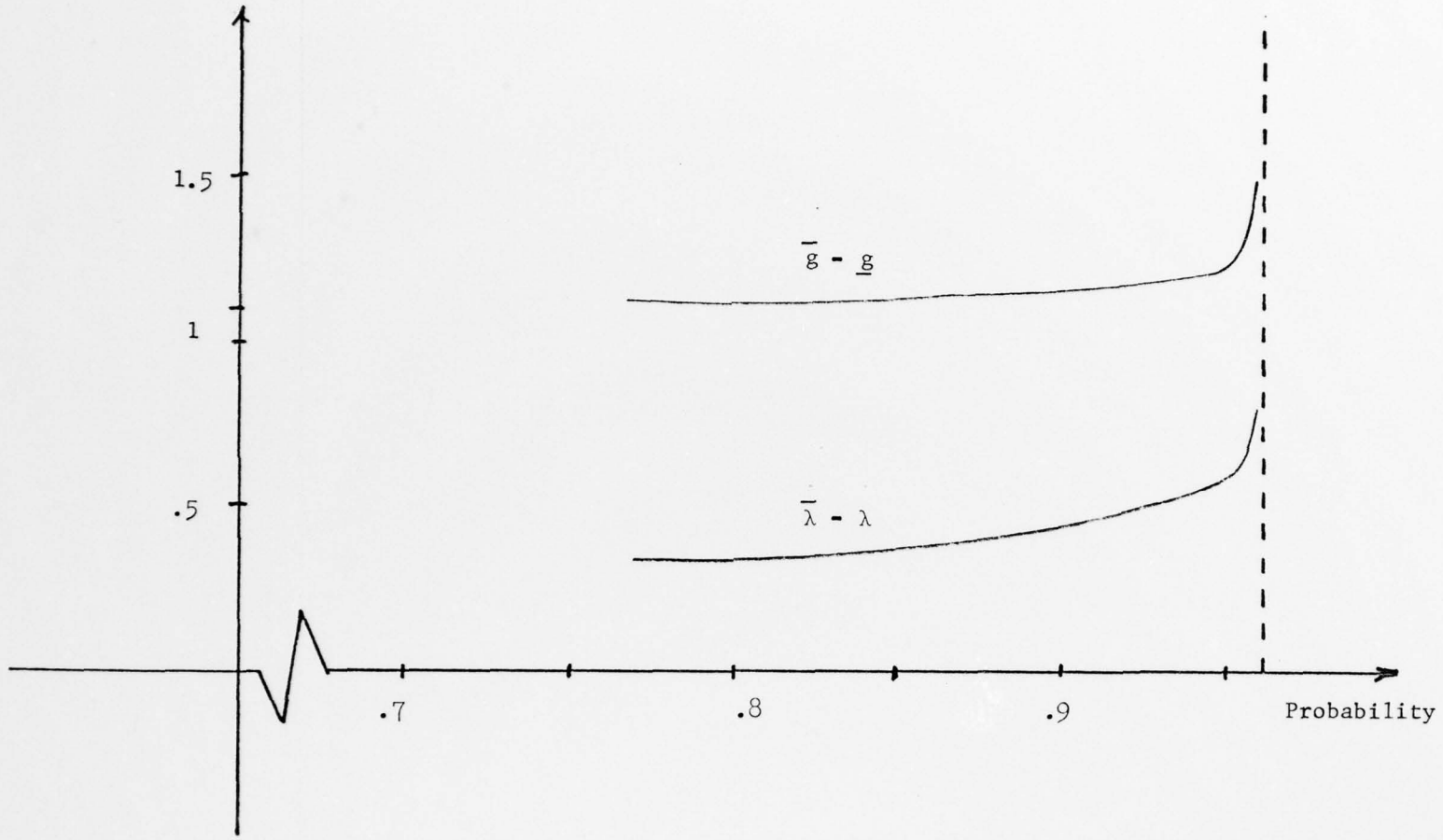

Figure 5. Region size vs. probability coverage when the observation at $\lambda = a_3$ is normally distributed.

There are two possible types of response to the situation when it turns out that $z_3(y) \geq 0$. The first response is based on the assumption that $g(\lambda)$ is actually a strictly concave function. In this case the analyst attempts to adjust the simulation results so as to obtain concave functions. The other type of response merely restricts the problem (1) to the closed interval $[a_0, a_{n+1}]$ where $a_0 \leq a_1$ and $a_{n+1} \geq a_n$ are user-specified constants. Of course, even a convex function attains a maximum over a closed bounded set. In the rest of this Section we discuss these two types of response in more detail.

The value of $z_3(y)$ will be negative as long as

$$A_j^1 > \frac{a_k - a_j}{a_k - a_i} A_i^2 + \frac{a_j - a_i}{a_k - a_i} A_k^2 \qquad (22)$$

for some $i < j < k$, $1 \leq i, j, k \leq n$. The adjustment process consists of modifying one triple A_i^2, A_j^1, A_k^2 if none of them satisfy (22). There are five ways to do this:

(1) By using the distribution theory that was used to obtain the original $[A_i^1, A_i^2]$ intervals, decrease the probability coverage (i.e., tighten the intervals) until (22) is satisfied. It may also be possible (if normal theory is applicable) to use asymmetric rather than symmetric intervals or to perform some other adjustement. It is likely that only a single interval will need to be altered.

(2) Carry out more simulation runs. These may be used to tighten the intervals already obtained or to investigate the response at an additional base point. Based on the results of this section, the

second alternative is suggested only when the responses at the existing points indicate that the optimum lies outside the current range.

(3) Inequality (22) may be expressed in terms of a constraint on y and explicitly introduced into the various optimization problems of Section 2 to insure that $z_3(y) < 0$. The main difficulty here is that (22) is a strict inequality; for this reason, a parameter $\mathscr{E}$ should be chosen and the following constraint used:

$$y_2 \geq \frac{a_3 - a_2}{a_3 - a_1} y_1 + \frac{a_2 - a_1}{a_3 - a_1} y_3 + \mathscr{E} \quad . \tag{23}$$

A good value for $\mathscr{E}$ would be a few percent of the maximum response obtained.

(4) The work of Barlow, et. al [1] on regression under order restrictions may be applied to adjust, say, A_1^2, A_2^1, and A_3^2 so that (22) always holds; this would involve estimates of the variability (i.e., variance) of the three values. This approach allows the analyst to use explicitly the additional information that $g(\lambda)$ is concave. This approach is somewhat involved and will not be discussed further here.

(5) The assumption that $g(\lambda)$ is concave may be questioned and a statistical test performed to determine its likelihood. This would involve information on the distribution of the simulation output response, however.

The constraint (23) offers a convenient means of carrying out the second approach, i.e. limiting the optimum λ^* to the interval $[a_0, a_{n+1}]$. In this case we solve for $\underline{\lambda}$ and $\overline{\lambda}$ as usual (the constraint protecting us from catastrophic unboundedness) and then set

$$\underline{\lambda} = \text{maximum } (a_0, \underline{\lambda})$$

$$\overline{\lambda} = \text{minimum } (a_{n+1}, \overline{\lambda}) \ .$$

As long as $\mathscr{E}$ is quite small this method should work well.

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This paper sets forth a method for finding a confidence region for the input parameter setting λ^* for which a system being simulated attains its optimum expected response, $g(\lambda^*)$. A confidence region for $g(\lambda^*)$ and a joint region for $(\lambda^*, g(\lambda^*))$ are also developed. The present work is restricted to the case where $g(\lambda)$ is a quadratic function of a single variable.

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